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The Modelling of Spills and Fumehood Containment in Laboratory Environments Using Large Eddy Simulations(LES)

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Outline

- Background: Lab Design Issues
- CFD Basics
- Turbulence: its influence & modelling
- Example
- Closing

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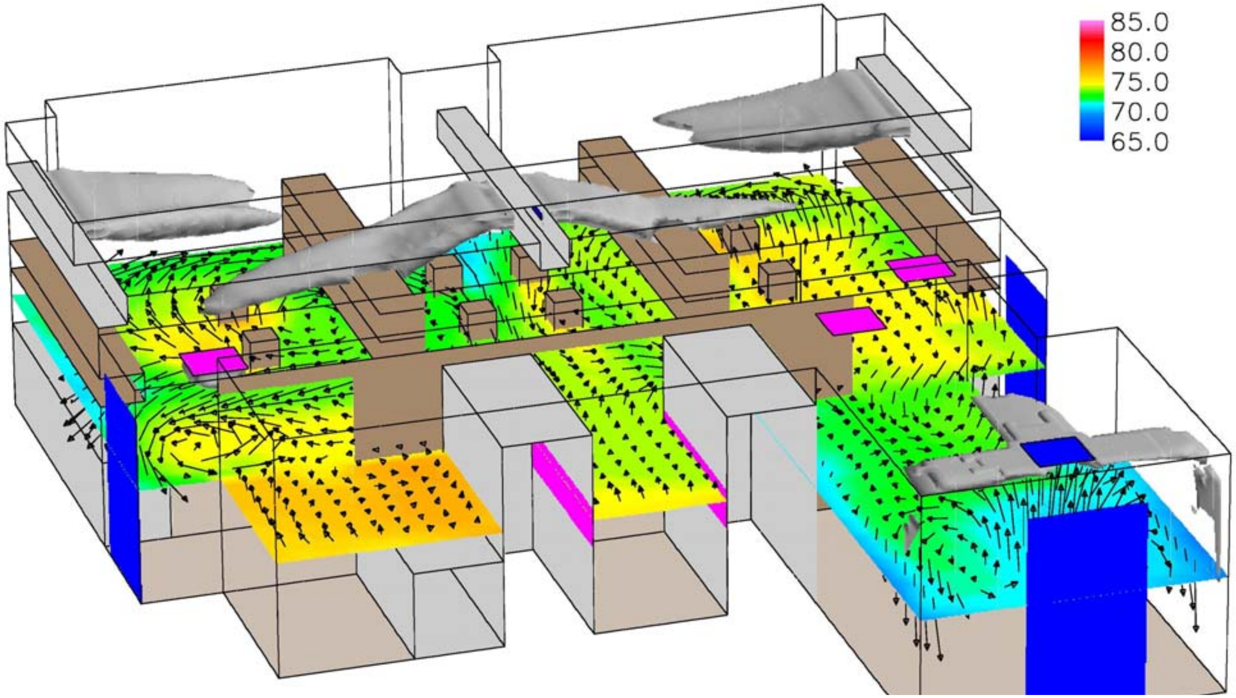
Background: Lab Design Issues
Why Simulate the Environment in a Lab

- Reduce ACH/minimize energy usage
- Optimize the return location – safety and ventilation efficiency
- Assess challenges to fumehood containment

Background: Flows in a Lab (Occupant Comfort)

- Temperature [ºF] and diffuser throw at 50 fpm



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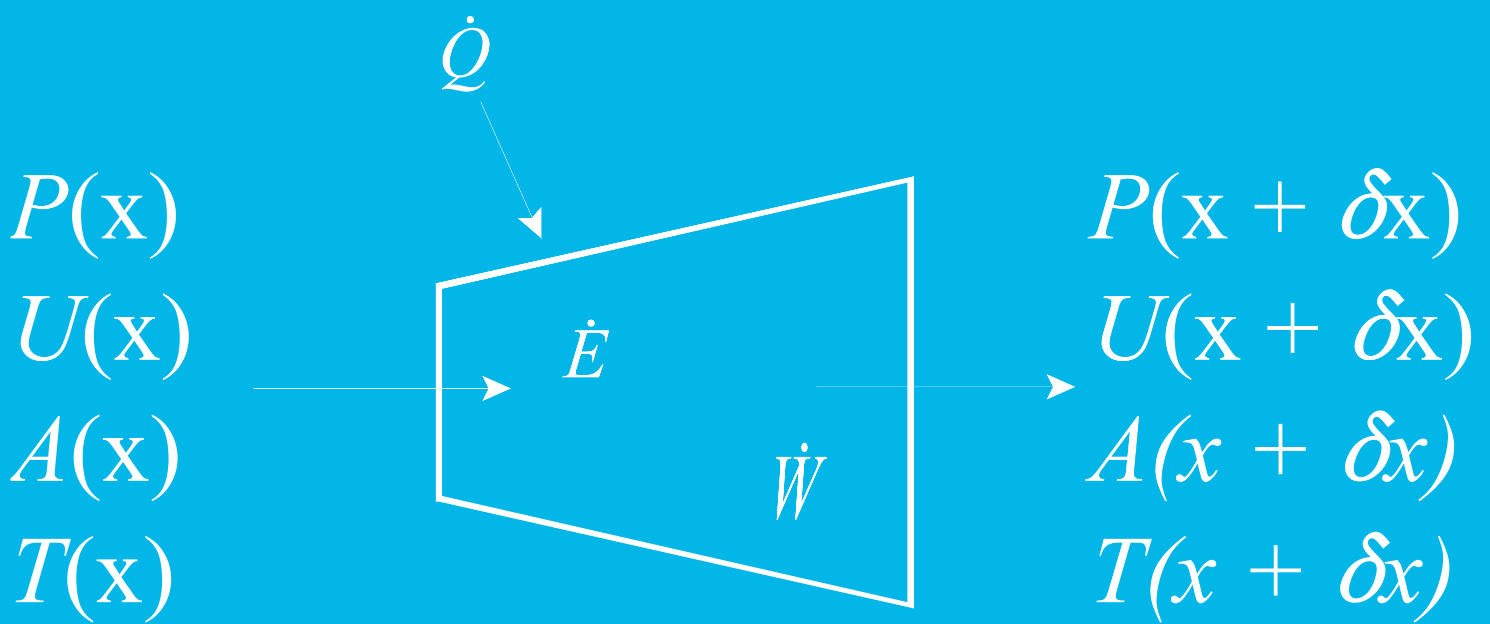
CFD Basics: How it Works

- One uses CFD to predict flow field properties by solving the Navier Stokes Equations



CFD Basics: What one Gets

- The solution of a CFD simulation in a typical laboratory generates a set of data for pressure, air speeds, temperature, turbulence quantities, and contaminant concentrations.

- These variables can be further analyzed to generate information such as fumehood capture challenges, occupant comfort, age of air/ventilation efficiency.

Turbulence: Its Role and Effects

- Turbulence is observed in most natural and engineering flows
- Turbulence is responsible for:
  - Increased heat transfer
  - Increased drag losses
  - Increased pollutant release from surfaces
  - Increased dispersion/transport of heat and contaminants about a space
- These effects can cause contaminants to escape from a fumehood and be rapidly transported about a lab

Turbulence: Modelling Difficulties

- Turbulence and the effects it causes represents a major uncertainty in CFD modelling.
- Difficulties are associated with the wide range of scale of turbulence – e.g. wind past a stack
  - The random appearance of small scales
  - The organized appearance of large scales
  - Small scales can represent sizable portion of total turbulence energy
- Other difficulties are geometry that causes flow separations, the methods by which turbulence is created & destroyed and the non-isotropic nature of it.

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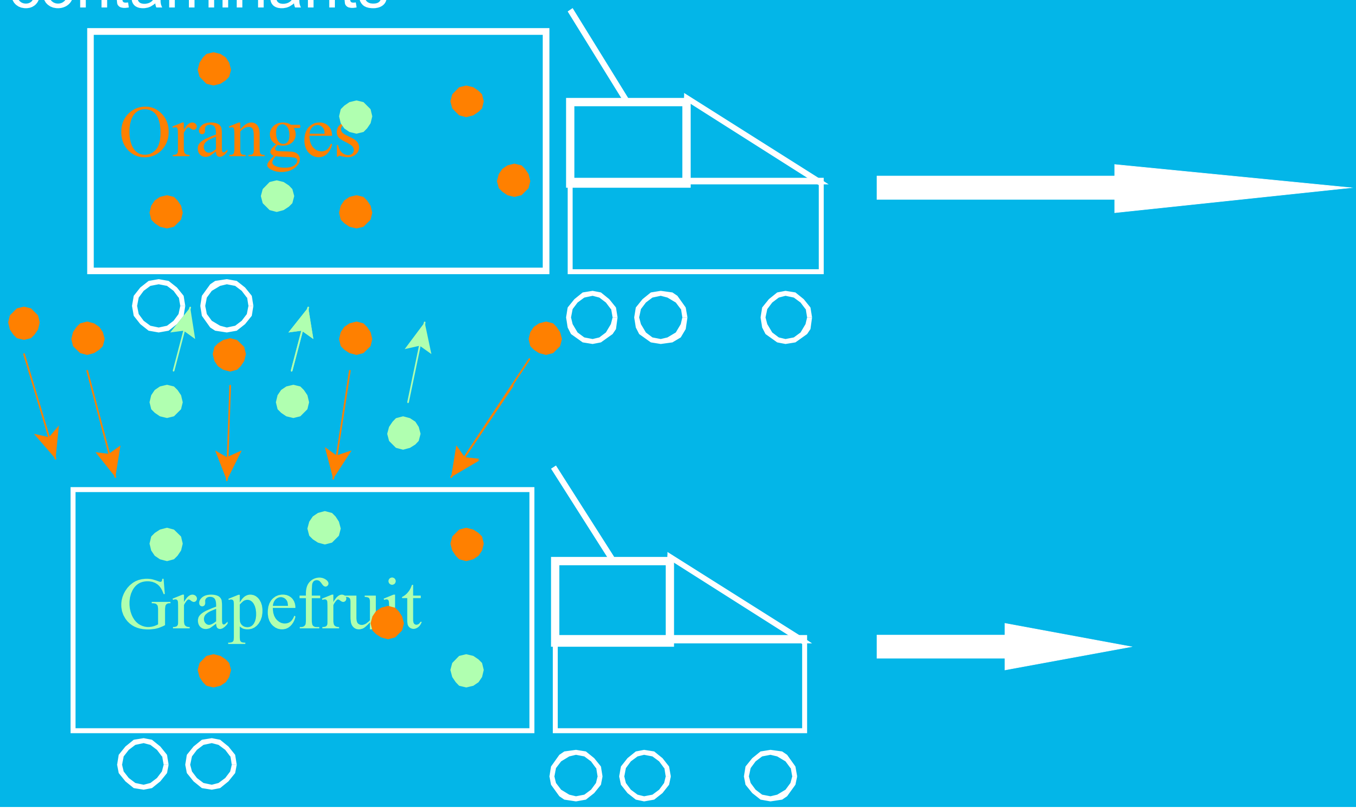
Turbulence: Modelling Options

- There are three main alternatives to modelling turbulence: the choice affects other modelling decisions.
  - DNS – Direct Numerical Simulation
    - Resolves smallest eddies
    - Computationally expensive
    - Currently unrealistic
  - RANS – Reynolds Averaged Navier Stokes
    - Provides prediction of “average” “steady” solution
    - The current method of choice
  - LES – Large Eddy Simulation
    - Resolves larger eddies and approximates smaller ones
    - Needs lots of cells near walls
    - Gaining attention
  - Detached Eddy Simulation (DES)
    - RANS near surfaces, LES further away
    - Coming … not yet

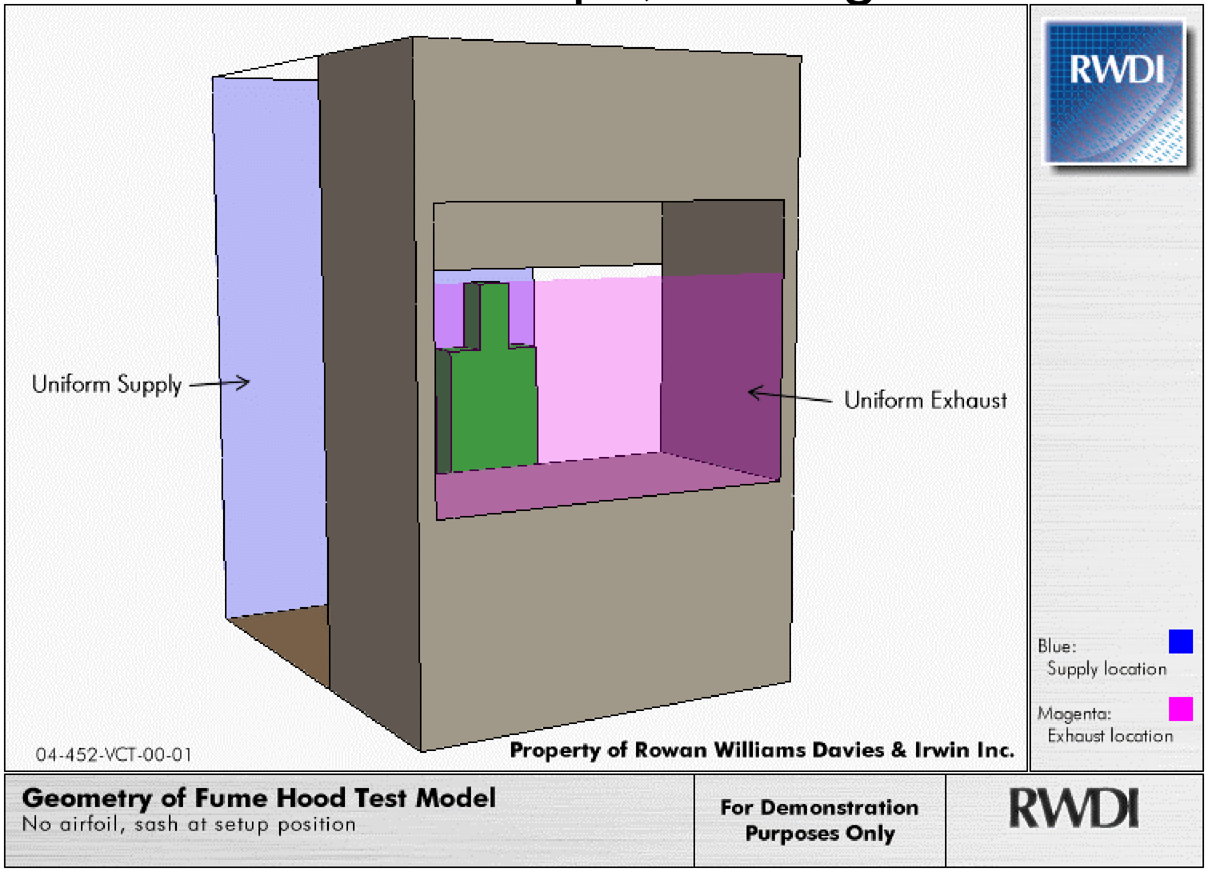
Turbulence Mechanisms

- Turbulent motion transporting packets of “information” – temperature, momentum, contaminants



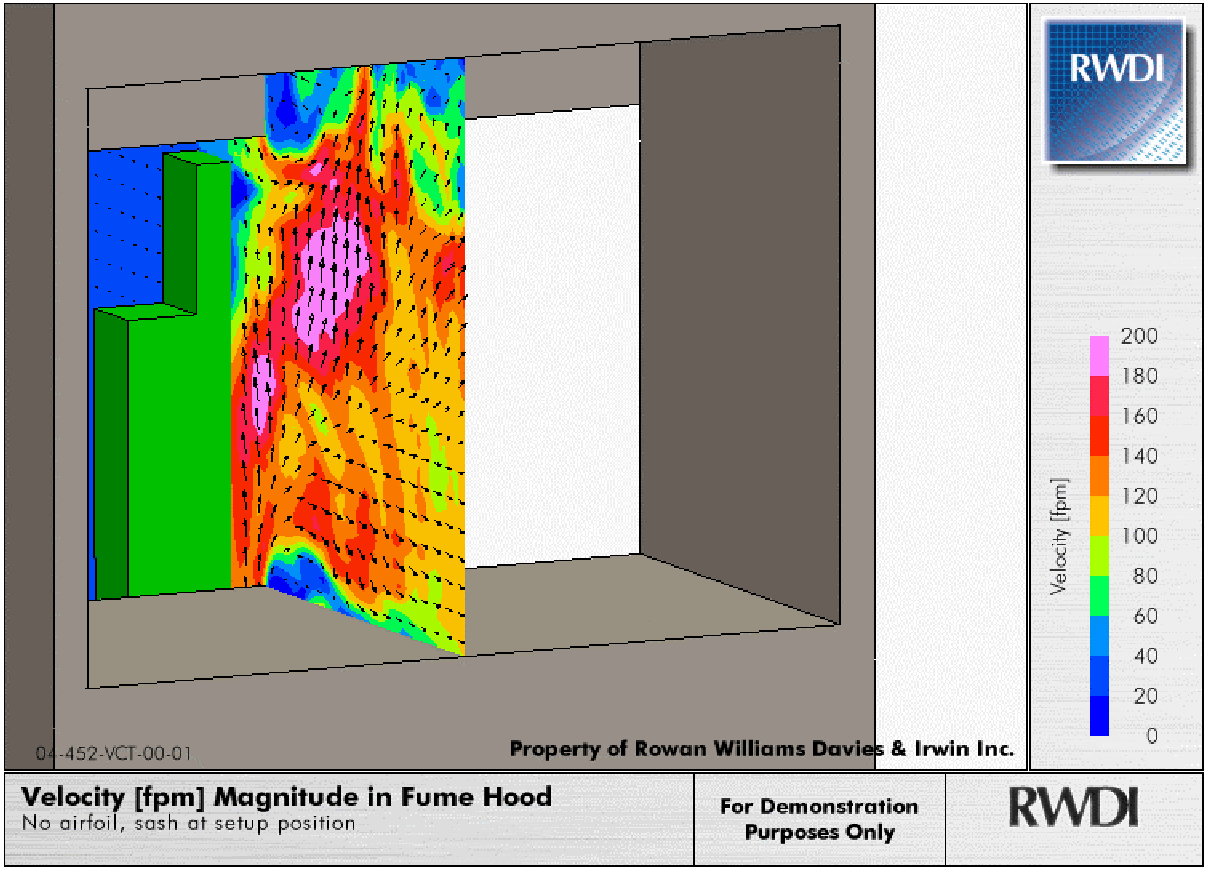
Turbulence: Test Fumehood Section

- Example CFD flow to show differences in LES and RANS – small time steps, small grid size



Turbulence: Test Fumehood in LES

- Animation shows detail



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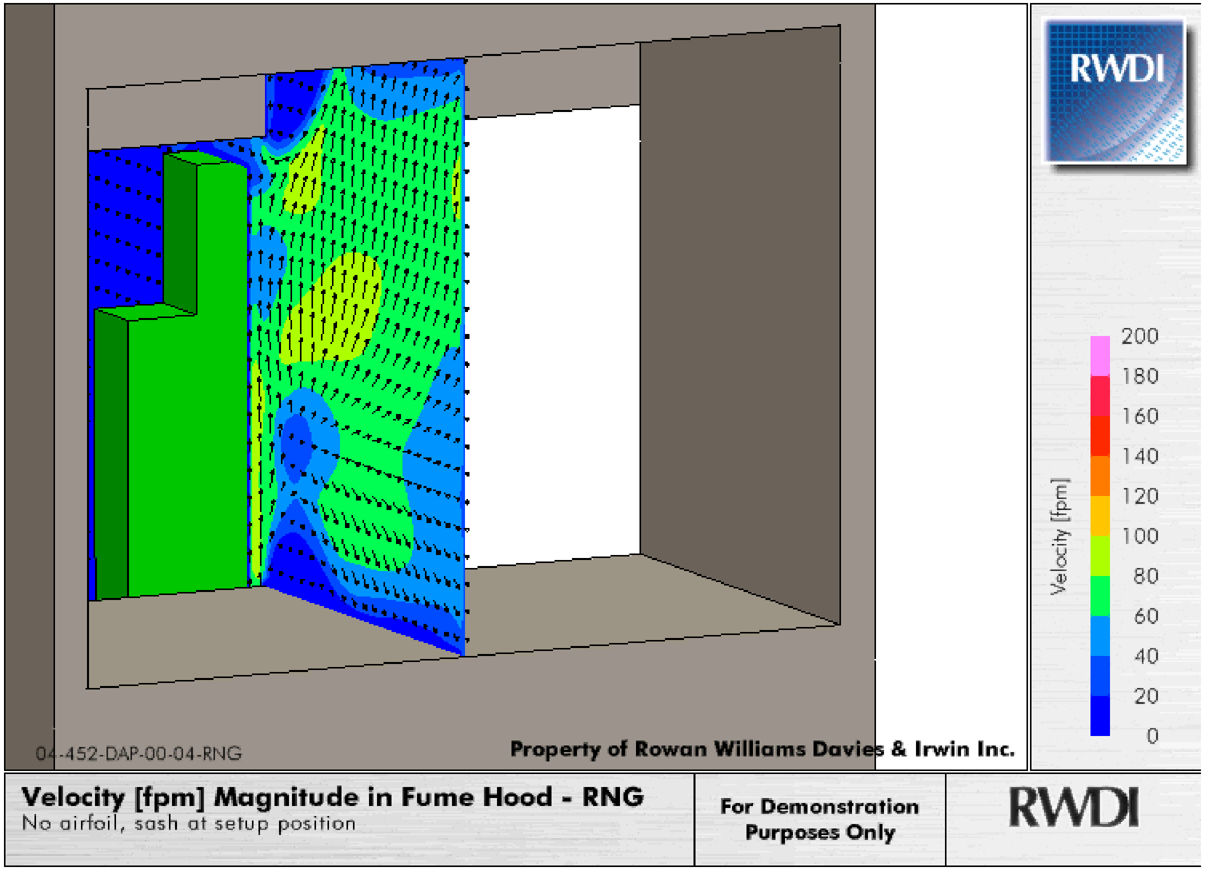
Turbulence: Test Fumehood in RANS

- Detail lost



Example

- Interested in exploring several issues:
  - What kind of benefit can be attained from return location
  - What is the influence of a reduced ACH

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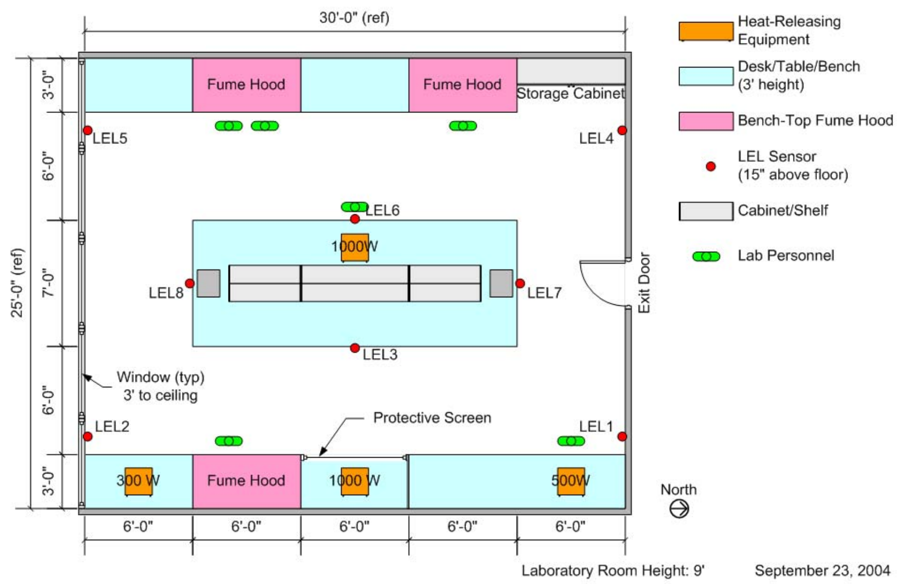
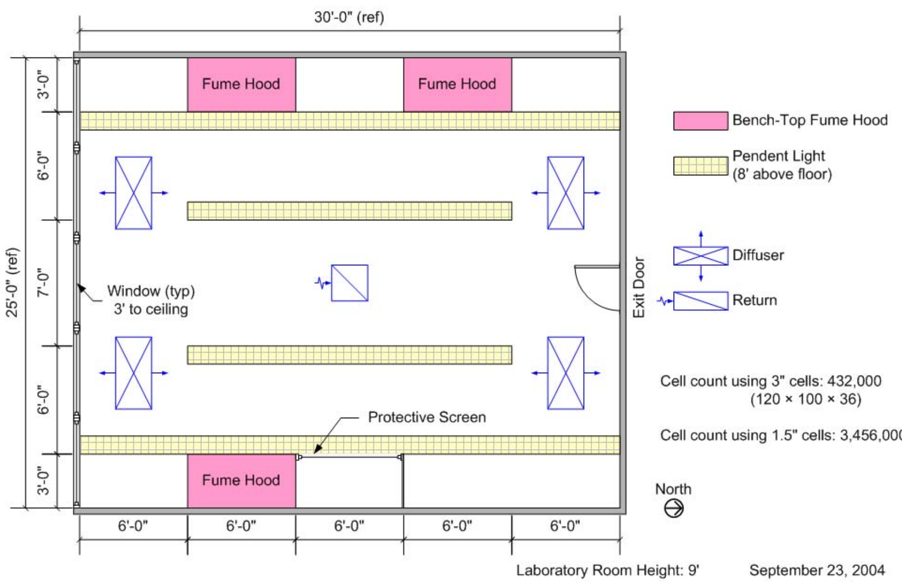
Geometry & Inputs

Test Laboratory Floor Plan



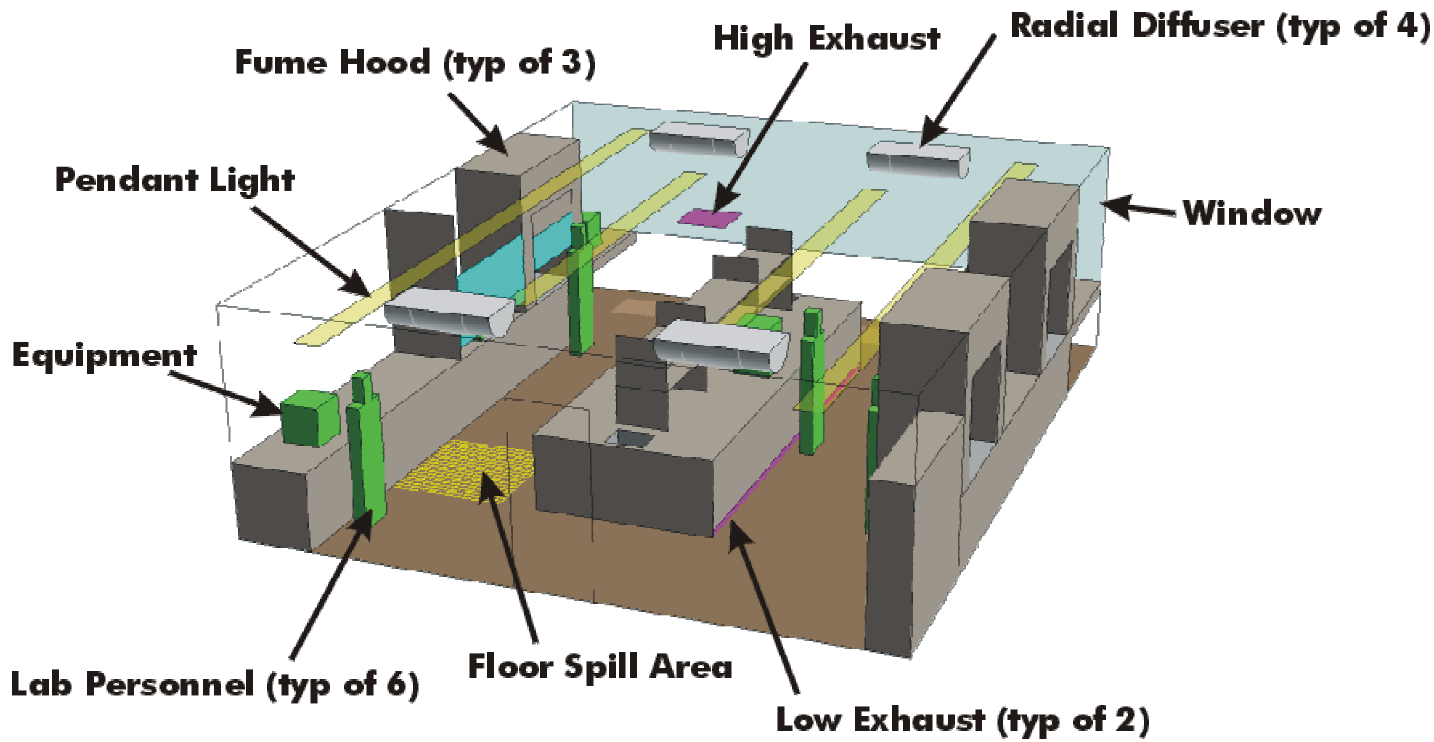
Test Laboratory Reflected Ceiling Plan



Cell count using 3" cells: 432,000
(120 × 100 × 36)

Cell count using 1.5" cells: 3,456,000

Geometry & Inputs



Boundary Conditions

- Scenarios
  - 20 ACH high return (nominal condition)
  - 20 ACH low return
  - 10 ACH high return

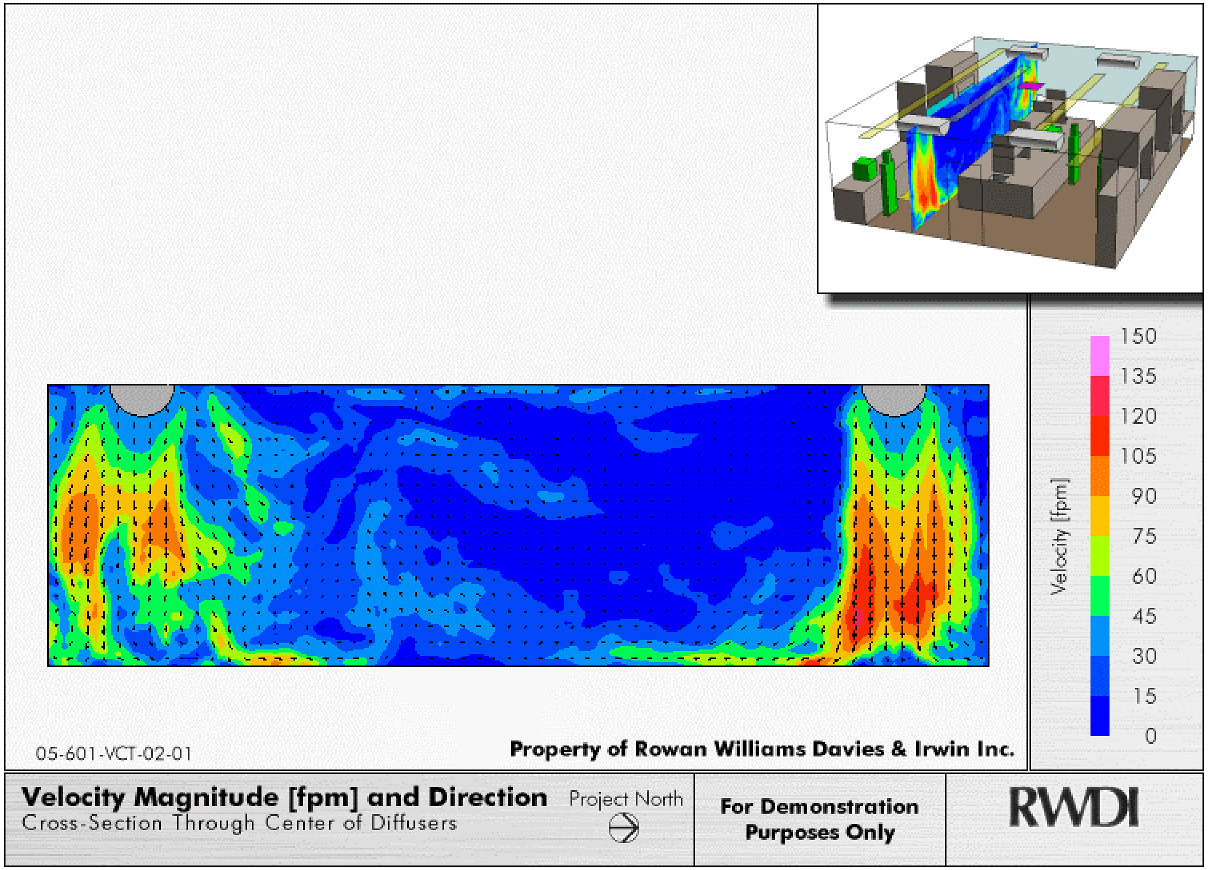
Flows

	20 ACH (2200 cfm)	10 ACH (1100 cfm)
Hood Exhaust	600 cfm * 3	333 cfm * 3
General Exhaust	450 cfm	125 cfm

- Heat Loads (7021 W total)
  - Lights 1.4 W/ft^2
  - Solar 2225 W
  - Equipment 2800 W total
  - People 450 W (75 W per person)

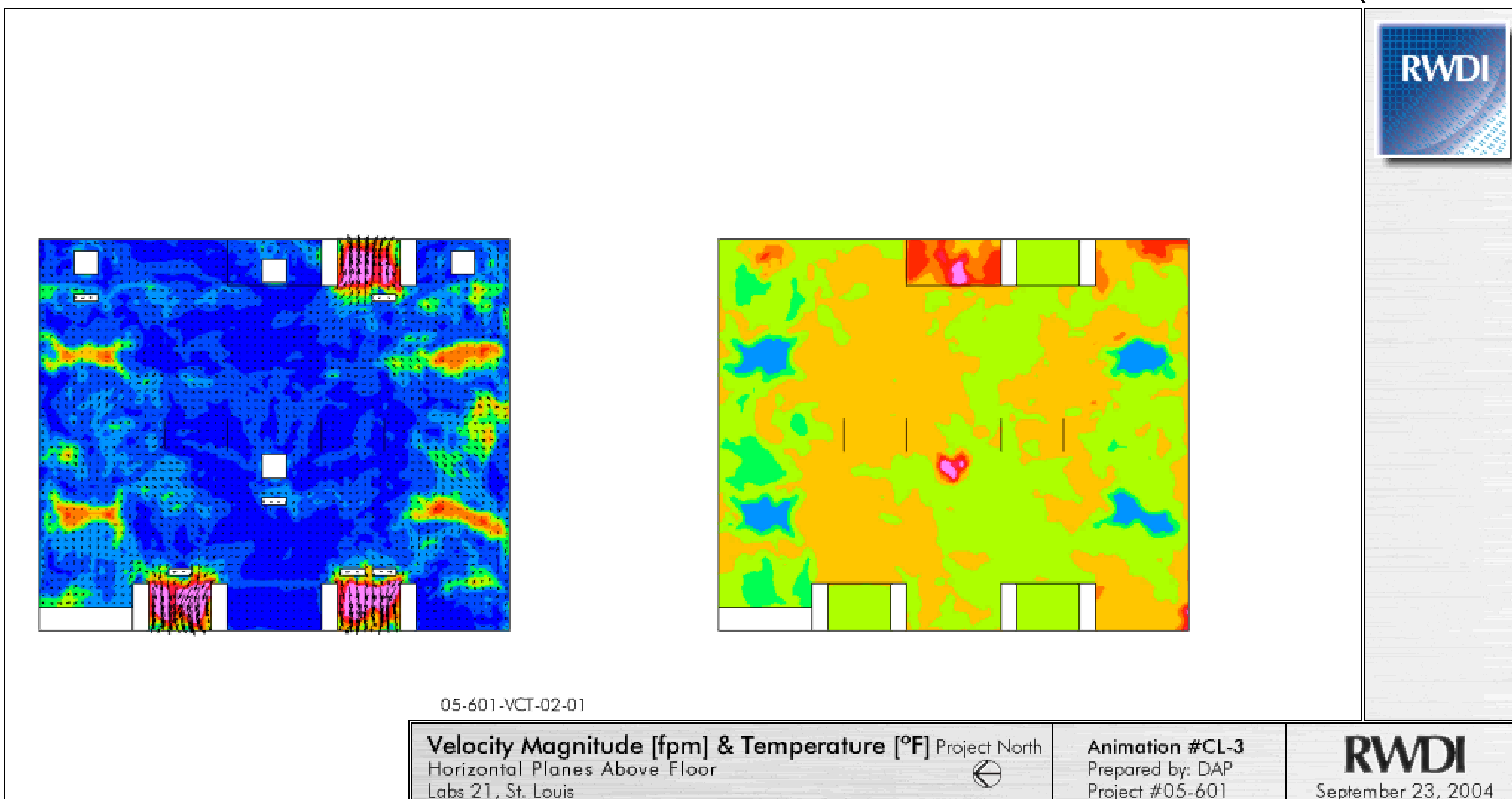
General Room Flows

- Animation shows:
  - Flow from diffuser & influence of solar load (window on RHS)



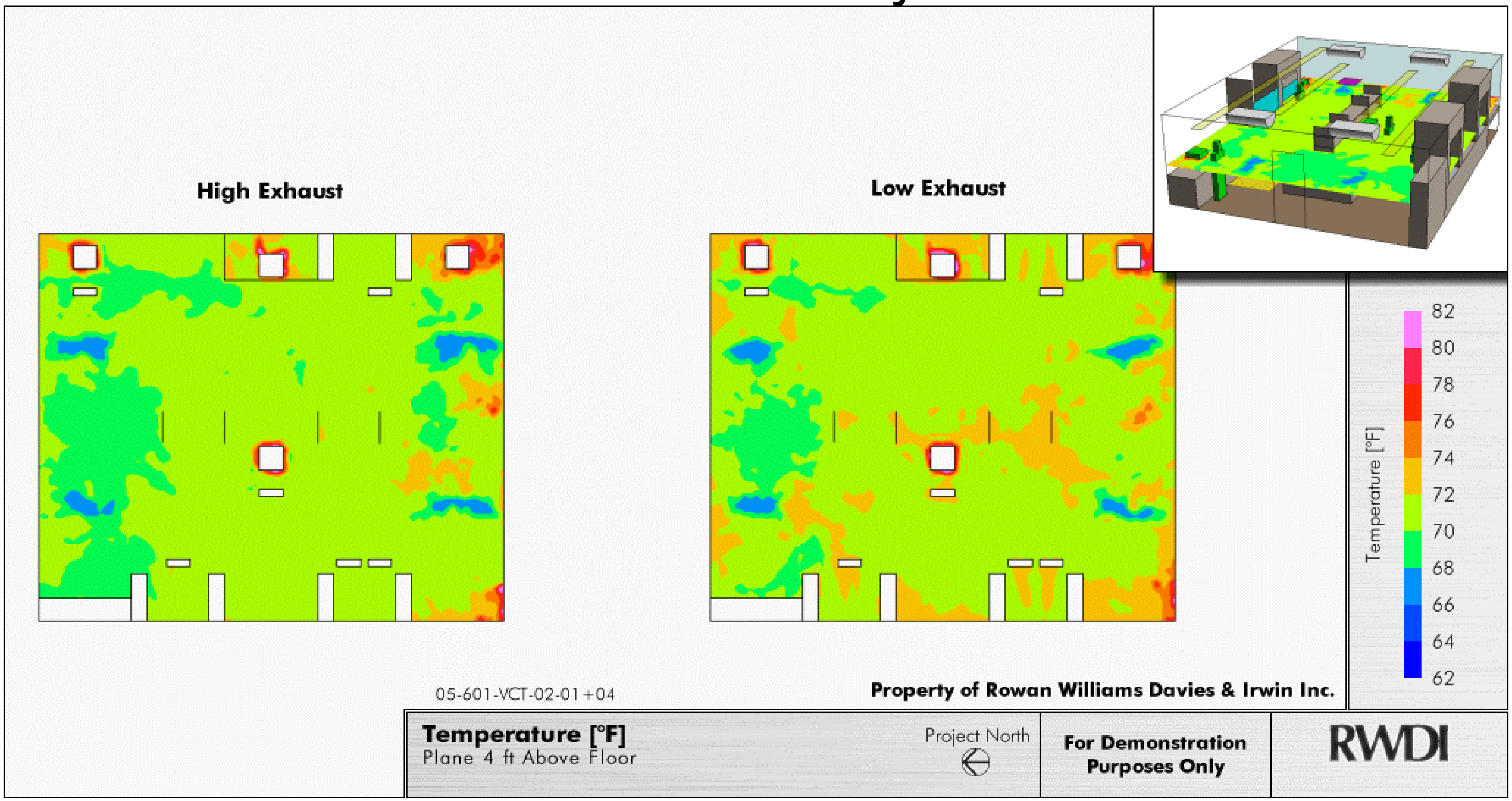
General Room Flows

- Animation shows:
  - Influence of solar load: flows near & far from window (at RHS)



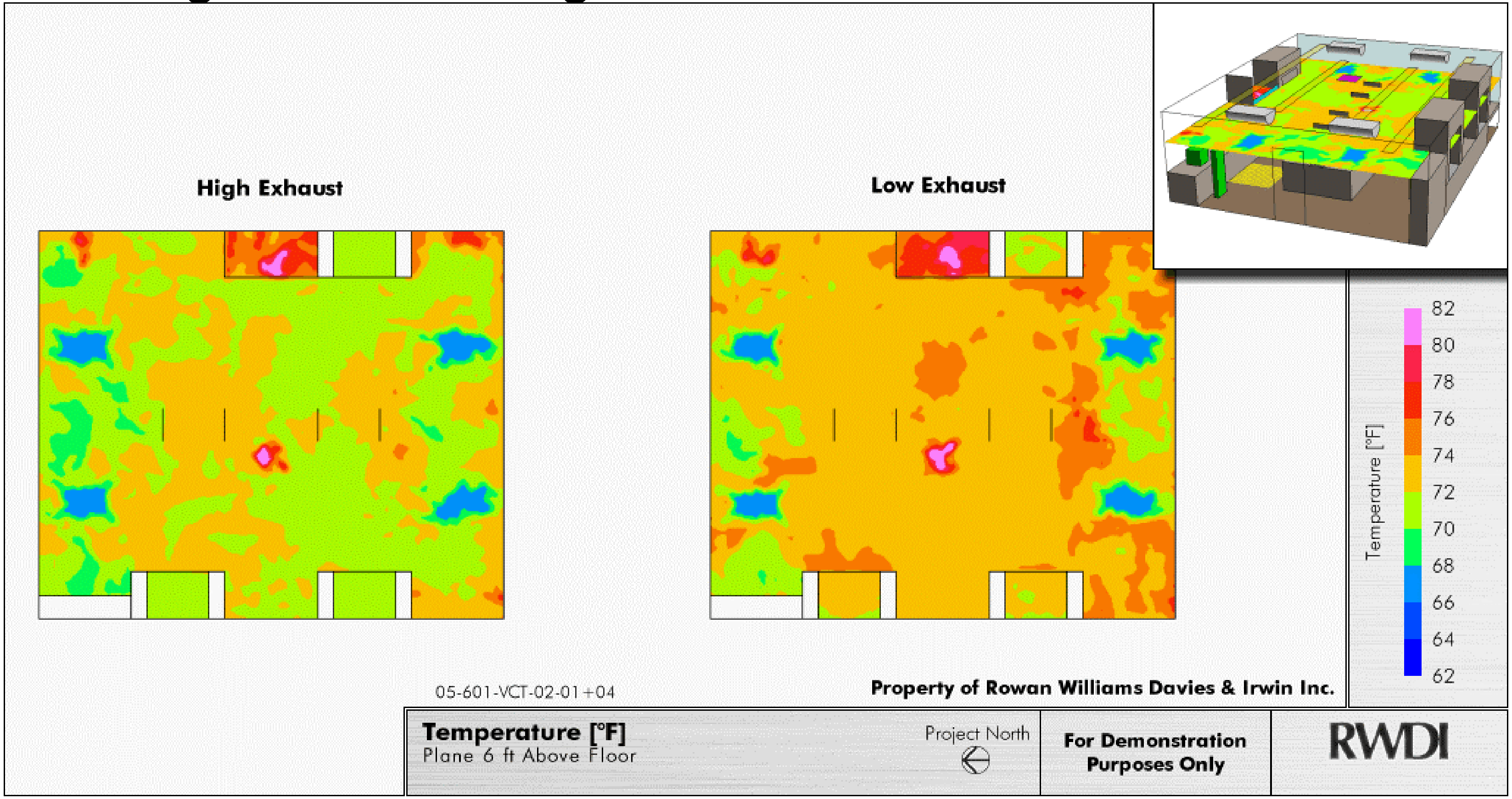
Comfort in Room: High vs. Low Return at 20 ACH

- Temperature at mid-body height similar: high return has cooler zone on LHS away from window



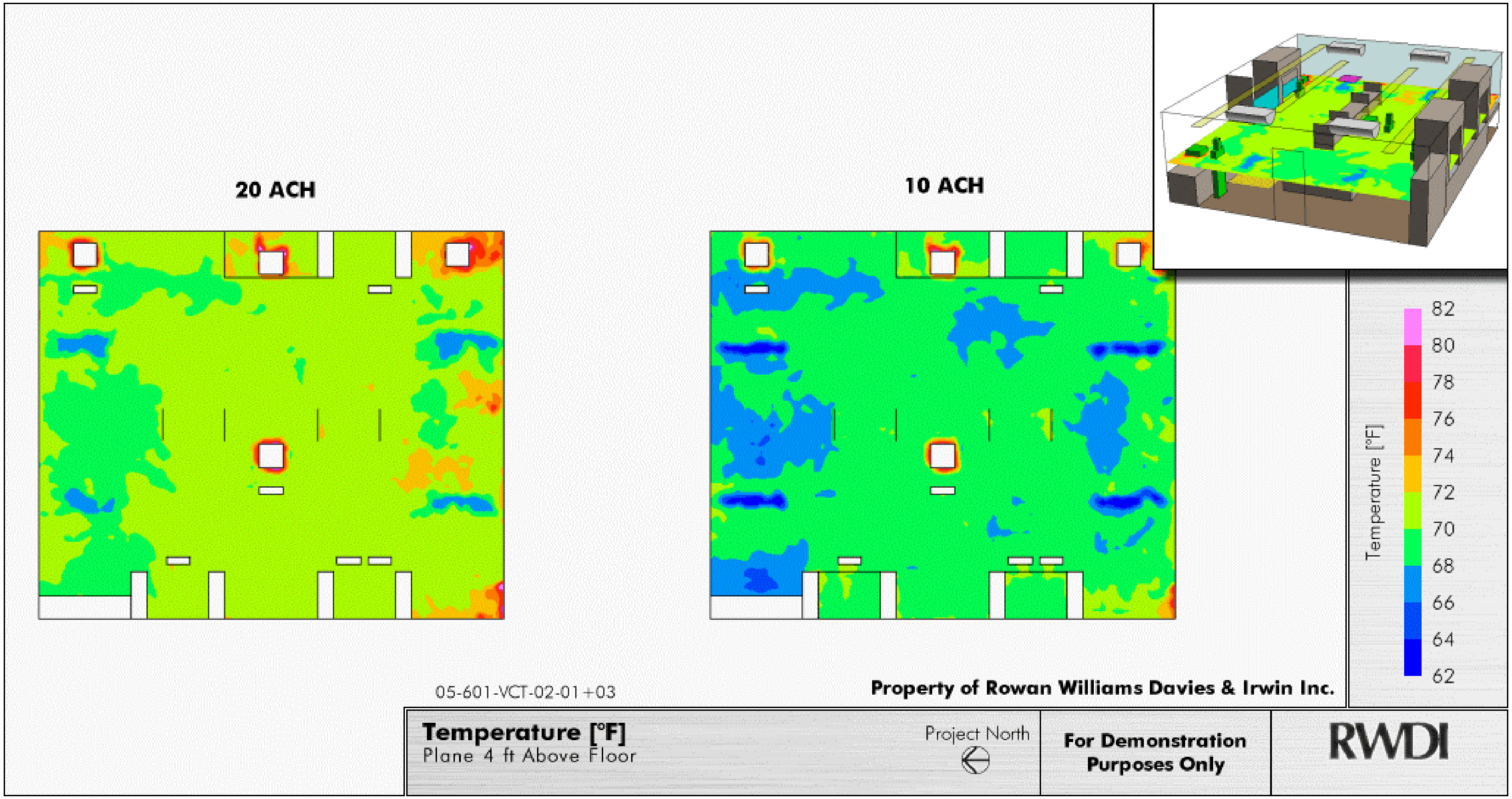
Comfort in Room:
High vs. Low Return at 20 ACH

- Stratification layer in low return case is lower than in high return configuration.



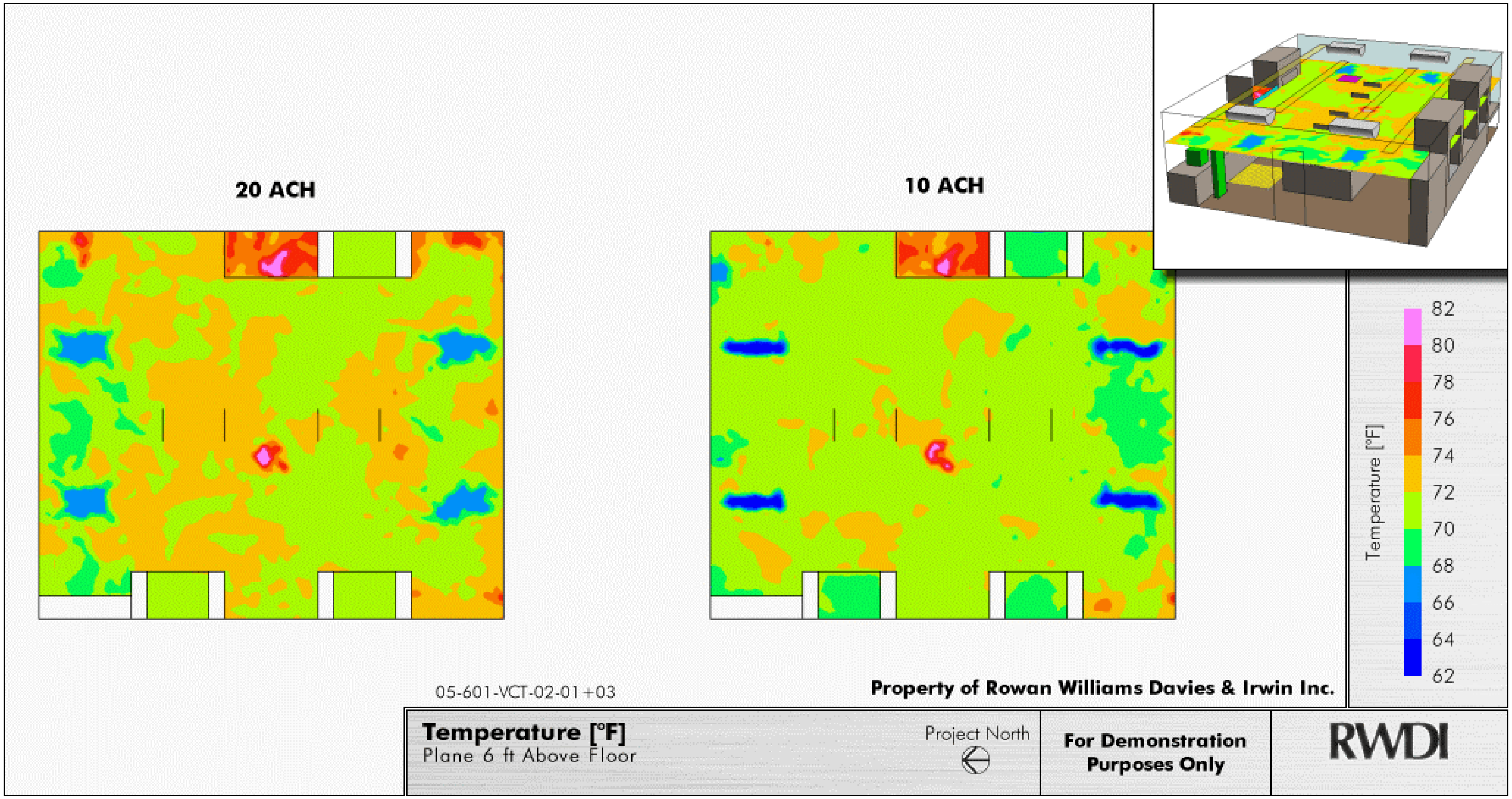
Comfort in Room: 20 vs. 10 ACH

- 10 ACH leads to localized cold zones at 4 ft



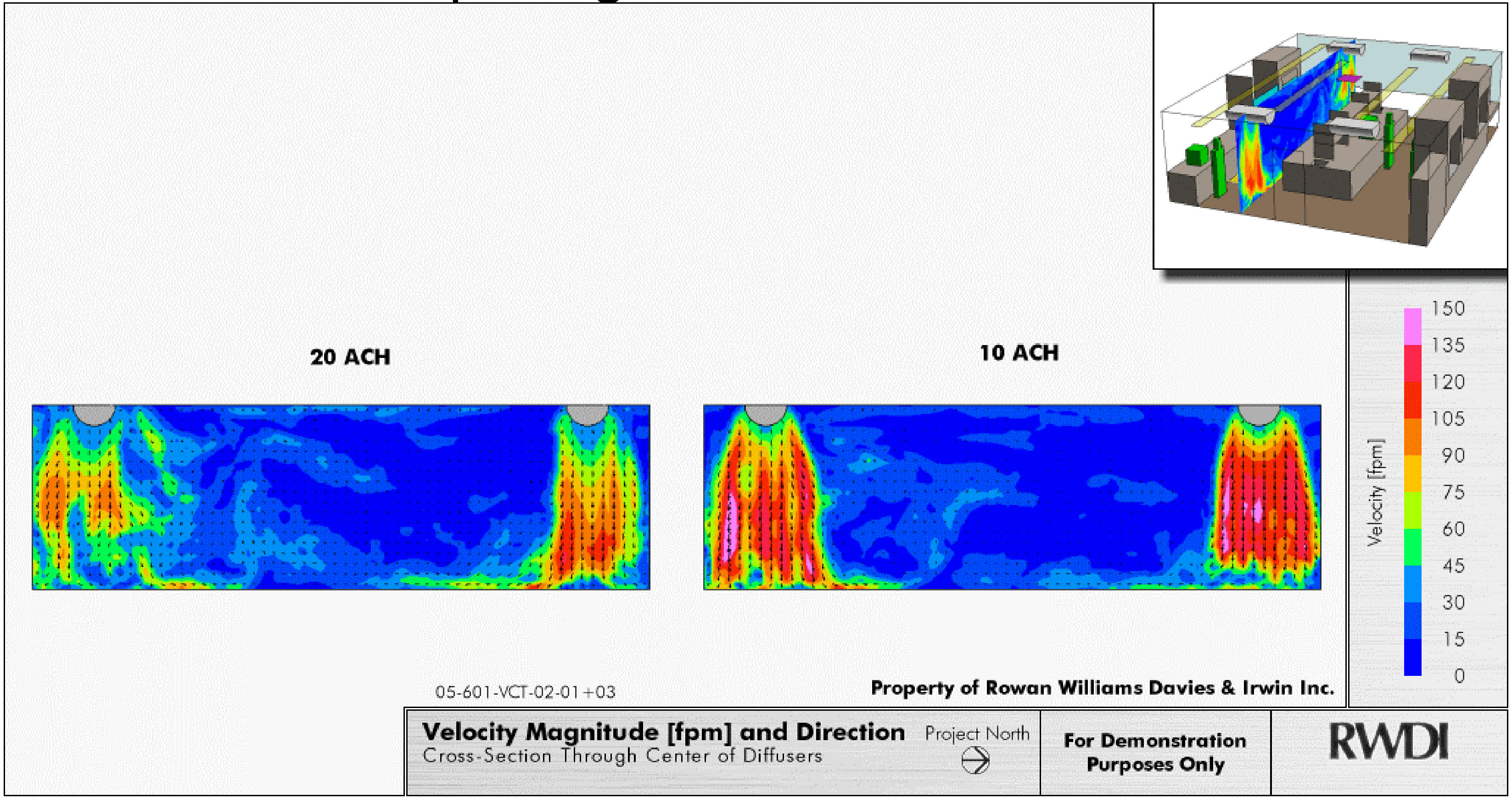
Comfort in Room: 20 vs. 10 ACH

- 10 ACH can result in better distribution at 6 ft



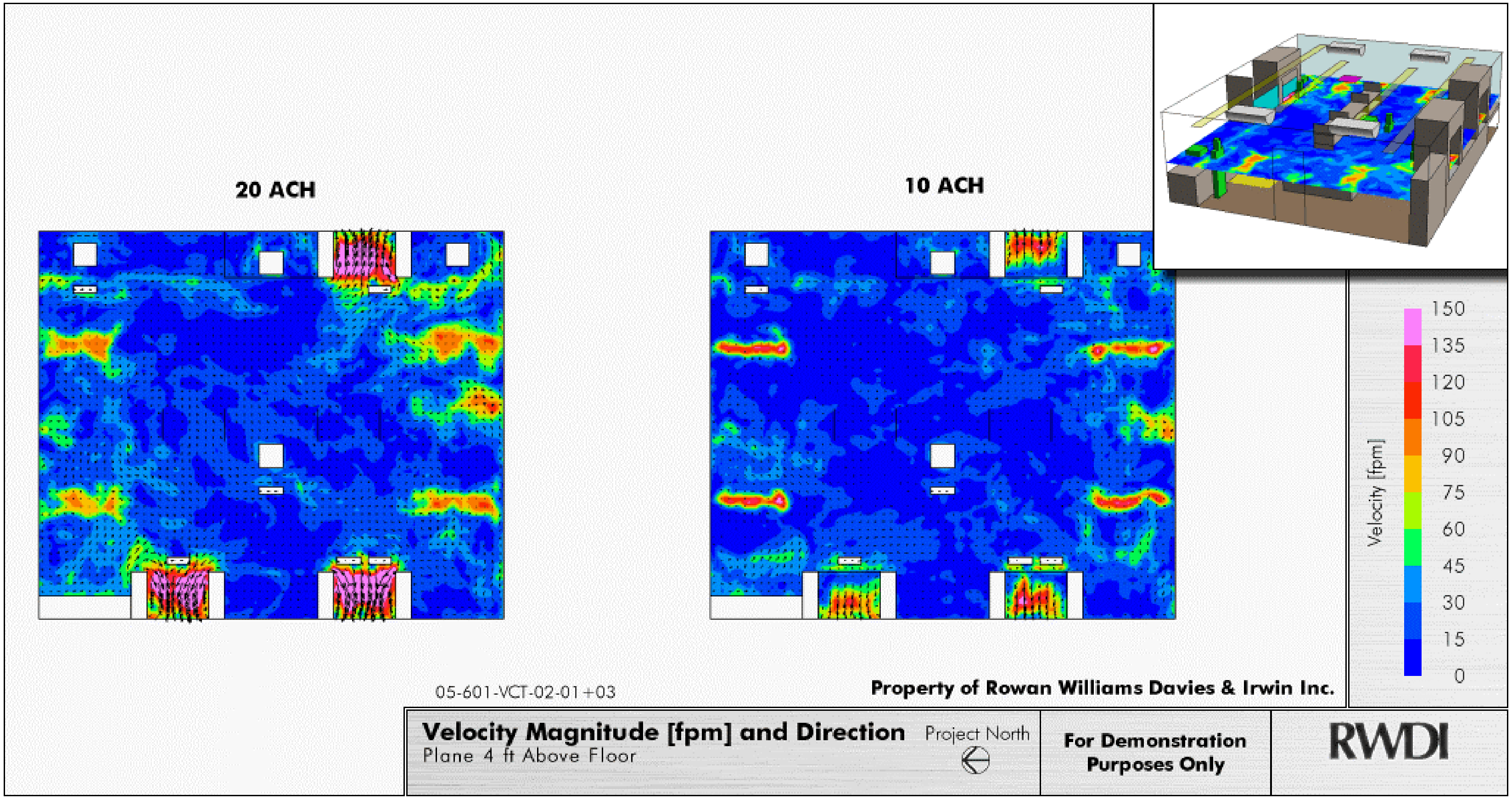
Fumehood Challenges: 20 vs. 10 ACH

- 20 ACH case can result in higher air speeds at fumehood opening level



Fumehood Challenges: 20 vs. 10 ACH

- Higher velocities arising from 20 ACH case can disturb flow near fumehood



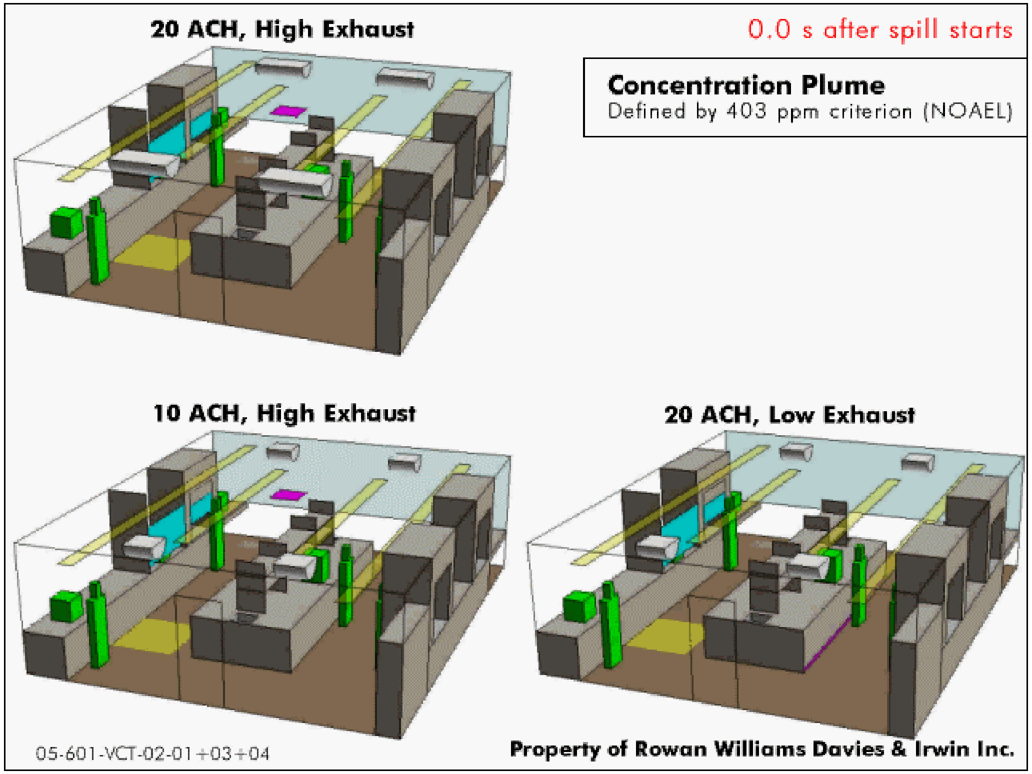
Safety: Evaluate the Influences of a Spill in the Lab

- Assume that a spill of MTBE occurs
  - Results in a heavy gas cloud forming near the floor
  - The setup of the ventilation system determines what will happen to the cloud
  - Can use this simulation technique to assess the concentration build-up to LEL, the risk of exposure, etc.

  - MTBE = Methyl tert-butyl ether

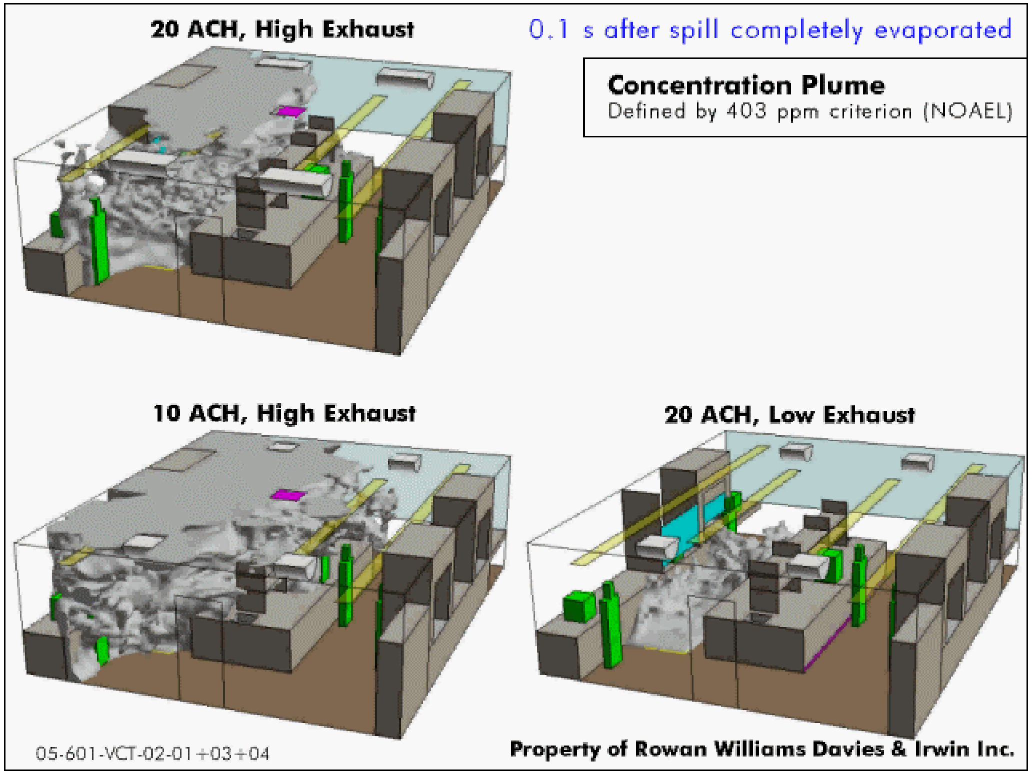
Safety: Transport of Gas About Room: Initial Stage

- Note ability of low return setup to reduce the spread about the room.
- NOAEL = no-observed-adverse-effect-level

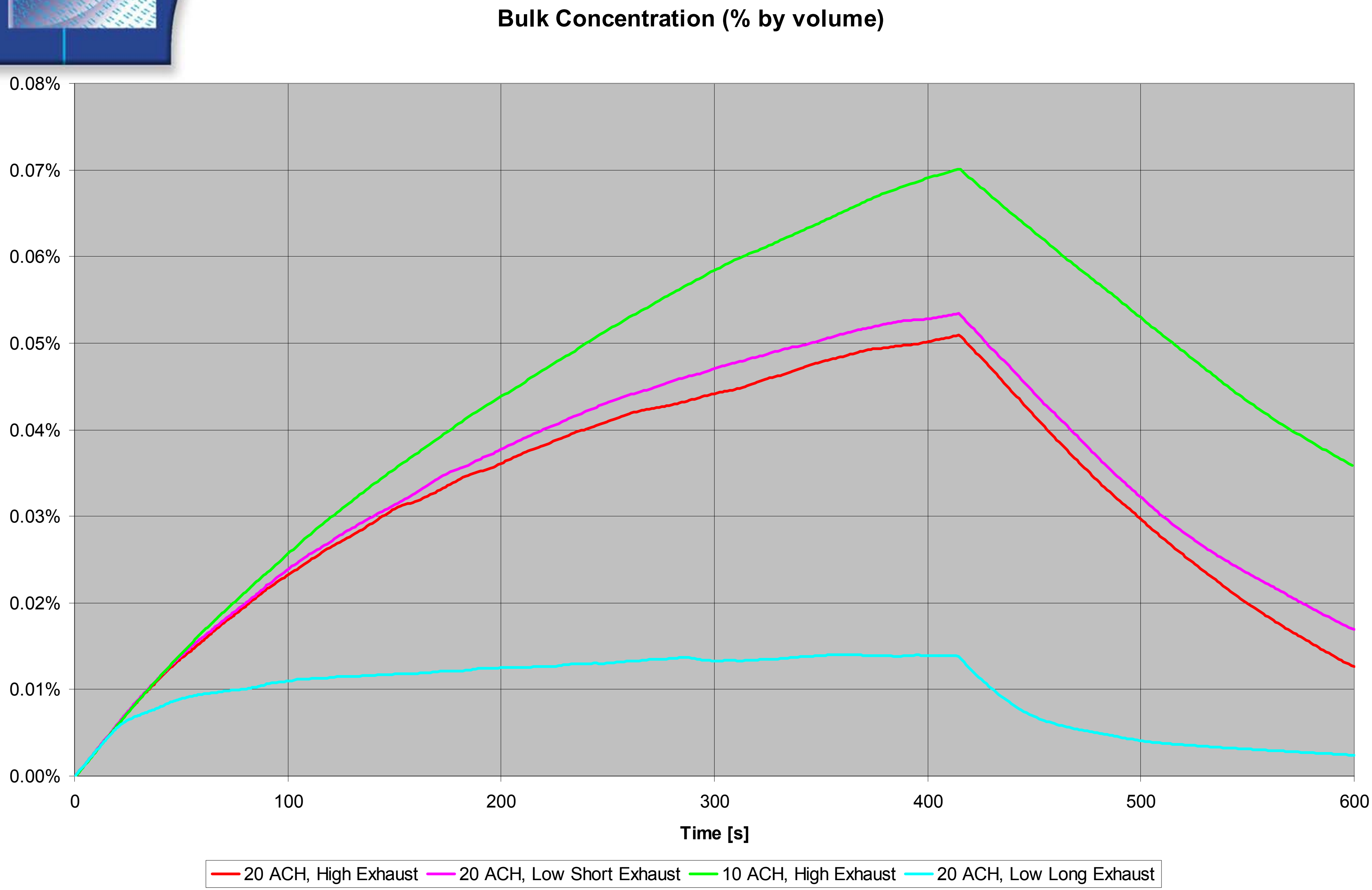


Safety: Transport of Gas About Room: After Full Evaporation

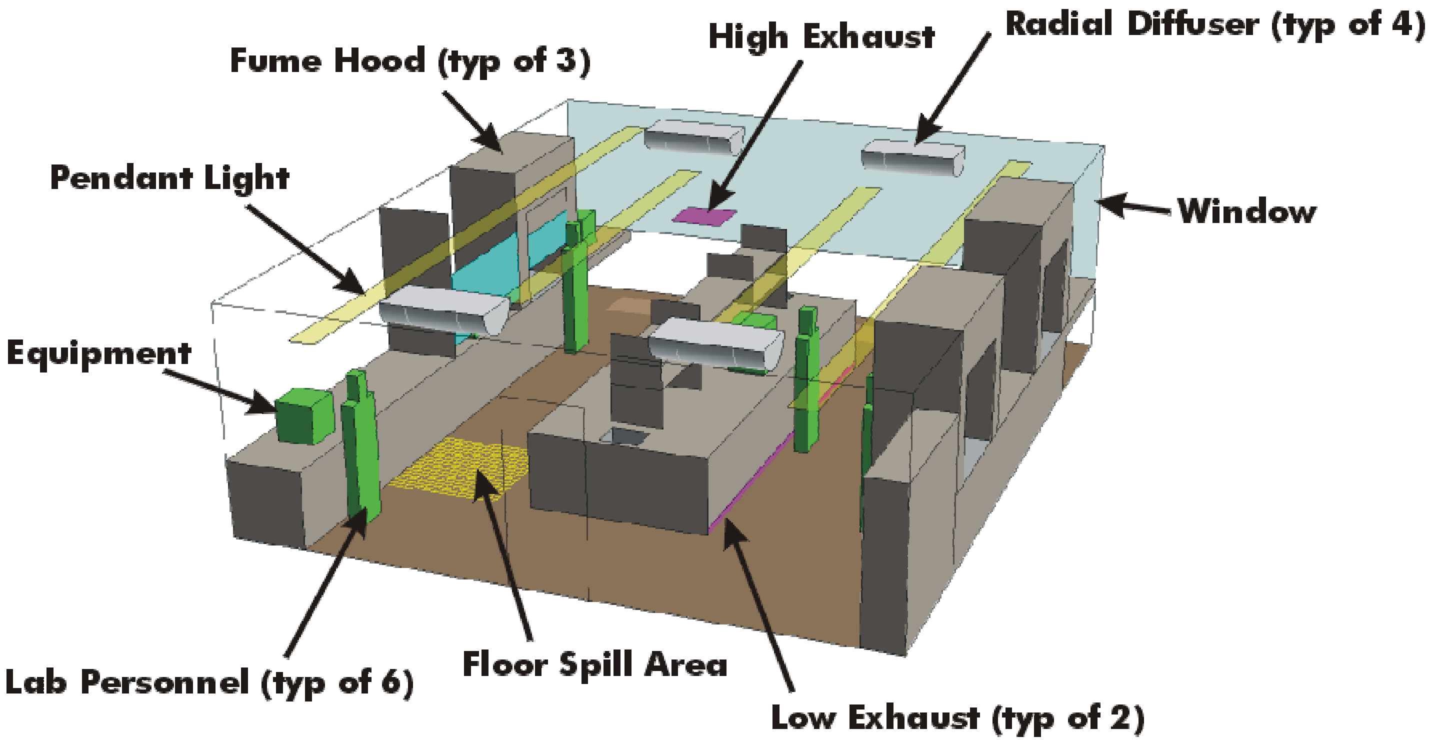
- The 1st frame of animation reflects worst conditions
- Low return flushes room quickly



Safety: Total Spill Vapour in Room



Safety: Location of Low Returns



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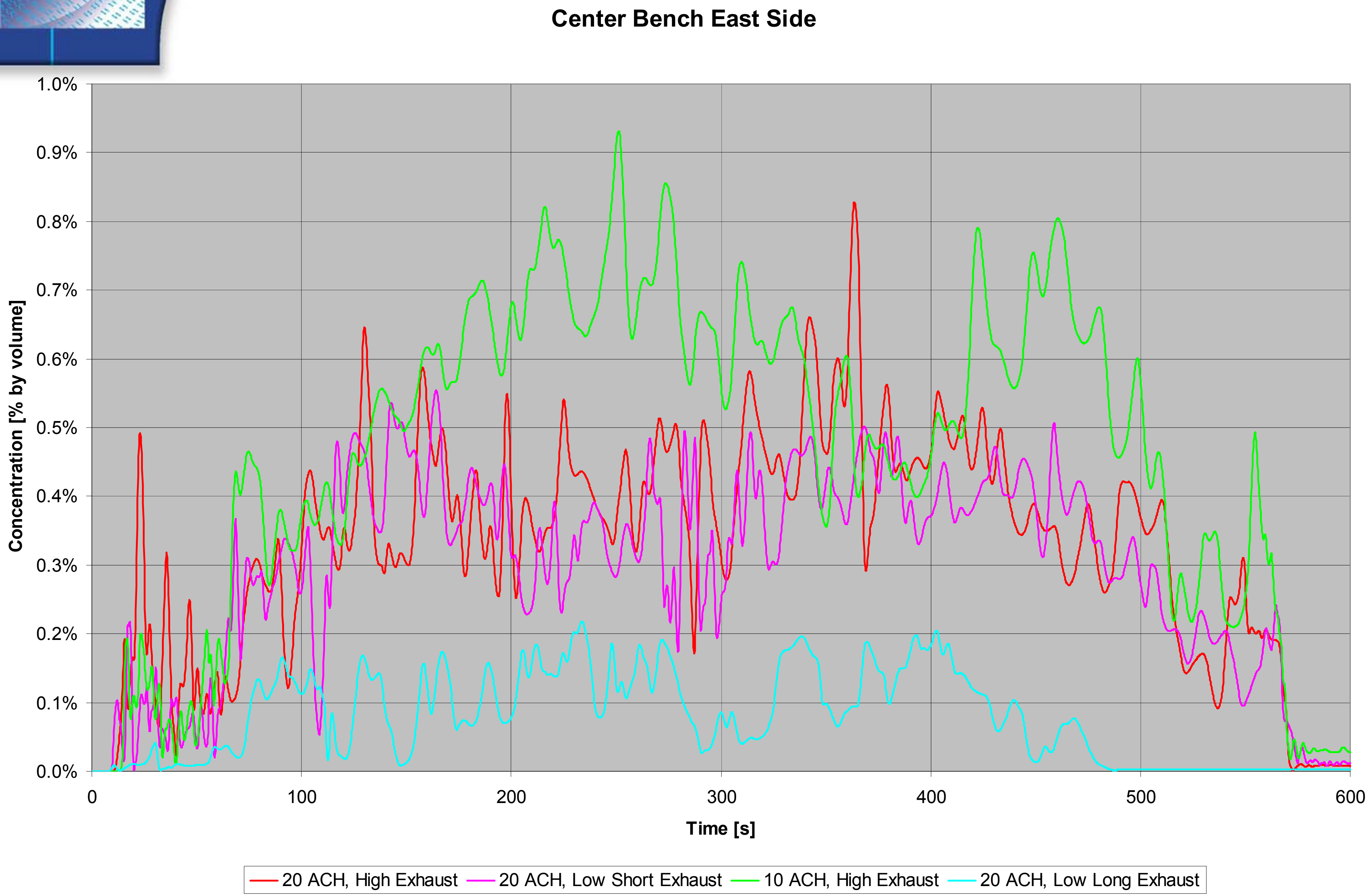
Safety: Build-up to LEL at Sensors



Findings from Work

- It is import to generally balance the supply and exhaust within a laboratory (not shown here);
- A higher air change rate (ACH) does not necessarily correlate to a safer laboratory; and,
- Fumehood containment can be challenged by the HVAC system setup.

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Labs 21 Approach : Advantages of Performing Early CFD

- Minimize overall environmental impacts
  - Impact of design changes intended to minimize energy use can be assessed in advance.
- Protect occupant safety
  - Both fumehood containment and a spill scenario are direct challenges to an occupant’s safety.
- Establish goals, track performance, and share results for continuous improvement
  - Comfort of an occupant within a space is important to their productivity. CFD simulations have been used to assess thermal comfort within laboratories to optimize worker comfort.